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Scientific Computation of Optimal Statistical Estimators

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14. ABSTRACT
The past century has seen a steady increase in the need of estimating and predicting complex systems and making (possibly critical) decisions with limited information. Although computers have made possible the numerical evaluation of sophisticated statistical models, these models are still designed by humans because there is currently no known recipe or algorithm for dividing the design of a statistical model into a sequence of arithmetic operations. With the purpose of addressing this problem this program has developed (1) the foundations of a rigorous framework for the scientific computation of optimal statistical estimators/models and (2) the required calculus enabling the reduction of optimization problems over measures over spaces of measures and functions. Two highlights of the work accomplished consist of (1) the application of the calculus to the identification of brittleness in Bayesian inference and (2) the application of the framework to the automated identification of scalable linear solvers for PDEs with rough coefficients.

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Scientific Computation of Optimal Statistical Estimators

Final Report

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Abstract: The past century has seen a steady increase in the need of estimating and predicting complex systems and making (possibly critical) decisions with limited information. Although computers have made possible the numerical evaluation of sophisticated statistical models, these models are still designed *by humans* because there is currently no known recipe or algorithm for dividing the design of a statistical model into a sequence of arithmetic operations. With the purpose of addressing this problem this program has developed (1) the foundations of a rigorous framework for the scientific computation of optimal statistical estimators/models and (2) the required calculus enabling the reduction of optimization problems over measures over spaces of measures and functions. Two highlights of the work accomplished consist of (1) the application of the calculus to the identification of brittleness in Bayesian inference and (2) the application of the framework to the automated identification of scalable linear solvers for PDEs with rough coefficients.

Summary of the work accomplished

Enabling computers to *think* as *humans* have the ability to do when faced with uncertainty is challenging in several major ways: (1) Finding optimal statistical models remains to be formulated as a well posed problem when information on the system of interest is incomplete and comes in the form of a complex combination of sample data, partial knowledge of constitutive relations and a limited description of the distribution of input random variables. (2) The space of admissible scenarios along with the space of relevant information, assumptions, and/or beliefs, tend to be infinite dimensional, whereas calculus on a computer is necessarily discrete and finite. This program has laid down the foundations for addressing these challenges by developing the required framework and calculus.

A framework for the scientific computation of optimal models/estimators. The framework, described in [14], consists of the full incorporation of *computation* and *complexity* into a natural generalization of Wald's Statistical Decision Function framework [23, 24, 25, 26, 27] (based on a generalization of Von Neuman's Theory of Games [21, 22]). In this framework optimal estimators/models are defined as optimal solutions of (minimax) adversarial games in which player A chooses the real system in an admissible set defined/constrained by available information and player B chooses the model/estimator, sees data generated by the real system and must predict some quantity of interest that is a function of the real system.

A calculus for manipulating infinite dimensional information structures. The resolution of these minimax problems require, at an abstract level, searching in the space of all possible functions of the data. By restriction models to the Bayesian class, the complete class theorem [27, 1, 3, 19] allows to limit this search to prior distributions on the admissible set of candidates for the real system, i.e. to measures over spaces of measures and functions. To enable the computation of optimal estimators this program has therefore identified conditions under which minimax problems over measures over spaces of measures and functions can be reduced to the manipulation of finite-dimensional objects and developed the associated reduction calculus. For min or max problems over measures over spaces of measures (and possibly functions) this calculus can take the form of a reduction to a nesting of optimization problems over measures (and possibly functions for the inner part) [16, 11, 17], which, in turn, can be reduced to searches over extreme points [18, 20, 2, 13]. Specific applications and developments of this calculus are as follows. [2] has presented sufficient conditions under which an Optimal Uncertainty Quantification (OUQ, [18]) problem can be reformulated as a finite-dimensional convex optimization problem, for which efficient numerical solutions can be obtained. The sufficient conditions include that the objective function is piecewise concave and the constraints are piecewise convex. In particular, it has been shown that piecewise concave objective functions may appear in applications where the objective is defined by the optimal value of a parameterized linear program. These developments have been applied in [2] to revenue maximization with stochastic supplies and to the optimal control of a power network with stochastic demands. The, more fundamental, results of [13, 12, 15] have laid down necessary steps for the identification of optimal reduced models on complex infinite-dimensional spaces (such reductions are ubiquitous with DFT and Navier-Stokes calculations). In particular, [13] has shown that, for the space of Borel probability measures on a Borel subset of a Polish metric space, the extreme points of the Prokhorov, Monge-Wasserstein and Kantorovich metric balls about a measure whose support has at most n points, consist of measures whose supports have at most $n + 2$ points. Moreover, using the Strassen and Kantorovich-Rubinstein duality theorems [13] has developed efficiently computable supersets of the extreme points. [12] has shown that for a Gaussian measure on a separable Hilbert space, the family of conditional measures associated with conditioning on a closed subspace are Gaussian with covariance operator the short of the covariance operator to the closed subspace. [15] has demonstrated that a reproducing kernel Hilbert space of functions on a separable absolute Borel space or an analytic subset of a Polish space is separable if it possesses a Borel measurable feature map.

Bayesian Brittleness. In the process of its development this calculus has been applied to analyse the robustness of Bayesian Inference under finite information [16, 11, 17, 10]. This analysis has uncovered the possible extreme sensitivity (brittleness) of Bayesian inference (in the TV and Prokhorov metrics or for Bayesian models that exactly capture an arbitrarily large number of finite-dimensional marginals of the data-generating distribution) and suggested that robust inference, in a continuous world under finite-information, should be done with reduced/coarse models rather than highly sophisticated/complex models (with a level of coarseness/reduction depending on the available finite-information) [17]. More precisely, although Bayesian methods are robust when the number of possible outcomes is finite or when only a finite number of marginals of the data-generating distribution are unknown, they appear to be generically brittle when applied to continuous systems (and their discretizations) with finite information on the data-generating distribution. Furthermore, if closeness is defined in terms of the total variation metric or the matching of a finite system of generalized moments, then (1) two practitioners who use arbitrarily close models and observe the same (possibly arbitrarily large amount of) data may reach opposite conclusions; and (2) any given prior and model can be slightly perturbed to achieve any desired posterior conclusions. The mechanism causing brittlenss/robustness suggests that learning and robustness are antagonistic requirements and raises the question of a missing stability condition for using Bayesian Inference in a continuous world under finite information.

Automation of the process of scientific discovery. In the process of developing this framework and calculus this program has started addressing (as a direct application of the framework and calculus) the fundamental question of whether scientific discovery can be computed, i.e., can the process of scientific discovery by guided by, or turned into an algorithm? (in some sense this question is related to that of whether machines can think). This program has addressed three notoriously difficult examples in which the answer to the above question is positive. The first one concerns the identification of new Selberg integral formulae [11] (a notoriously difficult problem of pure mathematics that has been turned into an algorithm). The second one concerns the identification of accurate, localized bases for numerical homogenization/coarse graining with optimal recovery properties [8] (a notoriously difficult problem of applied mathematics that has been turned into an algorithm). And the third one concerns the identification of near-linear complexity linear numerical solvers [9] (a notoriously difficult CSE problem that has been turned into an algorithm).

Gamblets. This latter example has lead the to the discovery of Gamblets [9] and shown that the discovery/design of scalable numerical solvers can be addressed/automated as a UQ problem by reformulating the process of computing with partial information and limited resources as that of playing underlying hierarchies of adversarial information games. As an illustration [9] has shown how the application of the proposed approach to the resolution of elliptic PDEs with rough coefficients leads to a near-linear complexity multigrid/multiresolution method with rigorous a-priori accuracy and performance estimates. In this application, the numerical solver has been discovered by identifying optimal strategies for gambling on the value of the solution of the PDE based on hierarchies of nested measurements of its solution or source term.

Development an efficient framework for heterogeneous computing and robust optimization This program has continued the development of (1) a computational job management framework (*pathos*) (a parallel graph execution framework providing a high-level programmatic interface to high-performance computing `http://trac.mystic.cacr.caltech.edu/project/pathos`, [5]) that offers a simple, efficient, and consistent user experience in a variety of heterogeneous environments from multi-core workstations to networks of large-scale computer clusters and (2) a robust optimization framework (*mystic*) (a highly-configurable optimization framework `http://trac.mystic.cacr.caltech.edu/project/mystic`, able to drive material science code to fit structures [6, 4]) that incorporates the mathematical framework described in [18, 7], and has provided an interface to prediction, certification, and validation as a framework service.

More precisely, under this program, asynchronous computing capabilities were added to pathos. Worker pools now provide asynchronous maps and pipes, as well as iterative ordered and unordered asynchronous variants. New asynchronous conditional parallel maps were added, which are both robust against failure and potentially orders of magnitude faster than blocking maps. Conditional maps terminate when the desired (potentially statistical) condition is met, as opposed to waiting for all results to return. The klepto package was created to provide an abstraction for storage and retrieval of objects in a database, in memory, or on disk. klepto provides asynchronous and distributed parallel caching (as opposed to recalculation) and cache interpolation strategies, and can be used to decouple the workflow and management of ASGs that span distributed resources. klepto also provides hierarchical caching, so for example a fast local cache could be maintained in memory with the most recently used entries, while a centralized global database serves as a second tier for all entries not interpolated or found in the fast local cache.

The majority of mystic was converted to asynchronous computing, thus enabling optimization to dramatically scale in size and complexity. Optimizers in mystic can now proceed in a step-by-step iterative fashion, potentially saving state at each step. This change enables mystic's optimizers to serve as a long-running daemon process that dynamically responds to new information – essentially optimizers have been converted to provide a "streaming" or "event" mode, to tackle real-time updates of information about the constraints or the cost function.

Given enough parallel resources, mystic's ensemble solvers demonstrate orders of magnitude improvements in speed and accuracy over industry standard genetic algorithms. With the addition of klepto, mystic's ensemble solvers were augmented to provide N-dimensional global search capabilities. For example, parallel ensembles of optimizers can be launched to search for all critical points and inflection points of an unknown surface, terminating only after no further points are found. The resulting points can then be fed into an N-dimensional interpolation engine, to produce a fast accurate surrogate model for the unknown surface.

Broader impact of the work accomplished. H. Owhadi and C. Scovel have been interviewed by HPC Wire[1]. The Bayesian Brittleness papers have generated significant blog activity[2]. Gamblets have been presented at a plenary lecture at SIAM CSE 2015[3]. H. Owhadi is co-editing "the Handbook of Uncertainty Quantification" (Springer) with R. Ghanem and D. Higdon. M. McKerns is editing a chapter in that book (on software aspects). H. Owhadi has been invited (by Dr. Bruce Suter DR-04 USAF AFMC AFRL/RITB) to AFRL, Rome NY to present and discuss the results of [9]. Schlumberger is exploring the incorporation of the results of [9] into its subsurface flows software. Gamblets have lead to a provisional patent (number 62/130,374).

[1] See www.hpcwire.com/2013/09/13/the_masters_of_uncertainty/

[2] See for instance http://errorstatistics.com/2015/01/08/on-the-brittleness-of-bayesian-inference-an-update-owhadi-and-scovel-guest-post/

[3] See https://www.pathlms.com/siam/courses/1043/sections/1259/thumbnail_video_presentations/9883

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Dr. Jean-Luc Cambier

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Abstract

The past century has seen a steady increase in the need of estimating and predicting complex systems and making (possibly critical) decisions with limited information. Although computers have made possible the numerical evaluation of sophisticated statistical models, these models are still designed \emph{by humans} because there is currently no known recipe or algorithm for dividing the design of a statistical model into a sequence of arithmetic operations. With the purpose of addressing this problem this program has developed (1) the foundations of a rigorous framework for the scientific computation of optimal statistical estimators/models and (2) the required calculus enabling the reduction of optimization problems over measures over spaces of measures and functions. Two highlights of the work accomplished consist of (1) the application of the calculus to the identification of brittleness in Bayesian inference and (2) the application of the framework to the automated identification of scalable linear solvers for PDEs with rough coefficients.

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- H. Owhadi, C. Scovel and T. Sullivan. Brittleness of Bayesian Inference under Finite Information in a Continuous World. Electronic Journal of Statistics, vol 9, pp 1-79, 2015.
- H. Owhadi and C. Scovel. Brittleness of Bayesian inference and new Selberg formulas. To appear in Communications in Mathematical Sciences (2015).
- H.Owhadi, L. Zhang and L. Berlyand. Polyharmonic homogenization, rough polyharmonic splines and sparse super-localization. ESAIM: Mathematical Modeling and Numerical Analysis. Special issue (2013).

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Dr. Jean-Luc Cambier DR-04 USAF AFMC AFOSR/RTA2 has replaced Dr. Fariba Fahroo AFOSR/RSL (now at DARPA)

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